Sensitivity and uncertainty analysis with the ERANOS code system

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Sensitivity and uncertainty analysis has played an important role in nuclear reactor analysis for more than forty years. Based on the pioneer work of Usachev and Gandini, computer codes have been developed in order to evaluate sensitivity coefficients based on perturbation theories already in the sixties, in particular in Europe. The ERANOS reactor analysis code system (Ref.1), has a wide range of capabilities to perform sensitivity and uncertainty analysis, and has been extensively used both for reactor physics and reactor design analysis. In the following paragraphs, it will be recalled a number of algorithms for very different applications (critical and sub critical reactors, fuel cycle physics etc). Examples will also be given of practical implementation in ERANOS.

1. Sensitivity Coefficients and Perturbation Theories

The variations of any integral parameter Q due to variations of cross sections σ can be expressed using perturbation theories (Ref. 2), to evaluate sensitivity coefficients S:

$$\delta Q/Q = \sum_j S_j \frac{\delta\sigma_j}{\sigma_j} \qquad (1)$$

where the sensitivity coefficients Sj are formally given by:

$$S_j = \frac{\partial Q}{\partial \sigma_j} \cdot \frac{\sigma_j}{Q} \qquad (2)$$

For practical purposes, in the general expression of any integral parameter Q, the explicit dependence from some cross-sections (e.g. σ_i^e) and the implicit dependence from some other cross-sections (e.g. σ_j^{im}) are kept separated:

$$Q = f(\sigma_j^{im}, \sigma_i^e). \qquad (3)$$

As an example, we consider a reaction rate:

$$R = \left\langle \underline{\sigma}^e, \underline{\Phi} \right\rangle \qquad (4)$$

where brackets $\langle , \rangle$ indicate integration over the phase space. In the case of a source-driven system, $\underline{\Phi}$ is the inhomogeneous flux driven by the external source, and the homogeneous flux in the case of critical core studies. In Eq. (4), $\underline{\sigma}^e$ can be an energy dependent detector cross-section; R is "explicitly" dependent on the $\underline{\sigma}^e$ and "implicitly" dependent on the cross-sections which characterize the system, described by the flux $\underline{\Phi}$. In other terms, R depends on the system cross-sections via $\underline{\Phi}$. Equation (1) can be rewritten as follows:

$$\delta Q / Q = \sum_j S_j \frac{\delta \sigma_j^{im}}{\sigma_j^{im}} + \left(\frac{\partial Q}{\partial \sigma^e} \cdot \frac{\sigma^e}{Q} \right) \cdot \frac{\delta \sigma^e}{\sigma^e} \tag{5}$$

where we have the hypothesis of an explicit dependence of Q on only one σ^e. If we drop the index "*im*":

$$\delta Q / Q = \sum_j S_j \frac{\delta \sigma_j}{\sigma_j} + \left(\frac{\partial Q}{\partial \sigma^e} \cdot \frac{\sigma^e}{Q} \right) \cdot \frac{\delta \sigma^e}{\sigma^e} = I + D \tag{6}$$

where the term I is generally called "indirect" effect, and the term D is called "direct" effect. While the direct effects can be obtained with explicit expressions of the derivatives of Q, the indirect effect (i.e. the sensitivity coefficients S), can be obtained with perturbation expression, most frequently at the first order (Ref. 2).

In what follows, we will explicit the formulations used by the ERANOS code system for the sensitivity coefficients at the first order for the indirect effects related to reactivity coefficients (Ref. 3), reaction rates (Ref. 2), nuclide transmutation (i.e., evolution in time, Ref. 4). The formulations related to other parameters of interest for critical or sub-critical systems will also be described (e.g. the reactivity loss during the irradiation, the effective fraction of delayed neutrons, the decay heat etc). These examples are provided in order to highlight the wide extent of capabilities of the sensitivity algorithms of the ERANOS code system..

1.1. Reactivity Coefficients (Ref. 3)

A reactivity coefficient (like the Doppler effect) can be expressed as a variation of the reactivity of the unperturbed system (characterized by a value K of the multiplication factor, a Boltzman operator M, a flux $\underline{\Phi}$ and an adjoint flux $\underline{\Phi}^*$):

$$\Delta\rho = \left(1 - \frac{1}{K_p}\right) - \left(1 - \frac{1}{K}\right) = \frac{1}{K} - \frac{1}{K_p} \tag{7}$$

where K_p corresponds to a variation of the Boltzmann operator such that:

$$\begin{aligned} M &\rightarrow M_p \left(= M + \delta M_p\right) \qquad \underline{\Phi} \rightarrow \underline{\Phi}_p \left(= \underline{\Phi} + \delta\underline{\Phi}_p\right) \\ \underline{\Phi}^* &\rightarrow \underline{\Phi}_p^* \left(= \underline{\Phi}^* + \delta\underline{\Phi}_p^*\right) \qquad K \rightarrow K_p \left(= K + \delta K_p\right) \end{aligned} \tag{8}$$

The sensitivity coefficients (at first order) for $\Delta\rho$ to variations of the σ_j are given as in Ref. 3:

$$S_j^{RO} = \frac{\partial(\Delta\rho)}{\partial\sigma_j} \cdot \frac{\sigma_j}{\Delta\rho} = \left\{ \frac{1}{I_f^p} \left\langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \right\rangle - \frac{1}{I_f} \left\langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \right\rangle \right\} \tag{9}$$

where $I_f = \left\langle \underline{\Phi}^*, F\underline{\Phi} \right\rangle$ and $I_f^p = \left\langle \underline{\Phi}_p^*, F\underline{\Phi}_p \right\rangle$, F being the neutron fission production part of the M (= F - A) operator.

1.2. Reaction Rates

The classical formulations found e.g. in Ref. 2 can be applied to the case of e.g., damage rate or He-production in the structures, or to the power peak factor in the core:

$$R = \left\langle \underline{\Phi}, \underline{\Sigma}_R \right\rangle \tag{10}$$

The sensitivity coefficients are given by:

$$S_j^R = \left\langle \underline{\Psi}_R^*, \sigma_j \underline{\Phi} \right\rangle \tag{11}$$

where $\underline{\Phi}$ has been defined above, and $\underline{\Psi}_R^*$ is the solution of:

$$M^* \underline{\Psi}_R^* = \underline{\Sigma}_R \tag{12}$$

and M^* is the adjoint of the operator M.

In the specific case of the power peak, this parameter can be expressed as the ratio:

$$R = \frac{\left\langle \Sigma_p \underline{\Phi} \right\rangle_{MAX}}{\left\langle \Sigma_p \underline{\Phi} \right\rangle_{Reactor}} \tag{13}$$

with Σ_p the power cross-section, essentially represented by $E_f \cdot \Sigma_f$, E_f being the average energy released per fission.

The sensitivity coefficients are defined as:

$$S_j = \left\langle \underline{\Psi}^*, \sigma_j \underline{\Phi} \right\rangle \tag{14}$$

and $\underline{\Psi}^*$ is the importance function solution of:

$$M^* \underline{\Psi}^* = \frac{\Sigma_{p,MAX}}{\left\langle \Sigma_p \underline{\Phi} \right\rangle_{MAX}} - \frac{\Sigma_{p,Reactor}}{\left\langle \Sigma_p \underline{\Phi} \right\rangle_{Reactor}} \tag{15}$$

where $\Sigma_{p,MAX}$ is the Σ_p value at the spatial point where $\langle \Sigma_p \underline{\Phi} \rangle \equiv \langle \Sigma_p \underline{\Phi} \rangle_{MAX}$, and $\Sigma_{p,Reactor}$ is the Σ_p value at each spatial point of the reactor. In Eq. (15) effects due to $\Sigma_{p,MAX}$ and $\Sigma_{p,Reactor}$ variations are assumed to be negligible.

1.3. Nuclide Transmutation (Ref.4)

The generic nuclide K transmutation during irradiation can be represented as the nuclide density variation between time t_0 and t_F. If we denote n_F^K the "final" density, the appropriate sensitivity coefficient is given by:

$$S_j^K = \frac{\partial n_F^K}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^K} = \frac{1}{n_F^K} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \; dt \tag{16}$$

where the time dependent equations to obtain $\underline{n}^*$ and $\underline{n}$, together with their boundary conditions, are defined in Ref. 4.

1.4. Reactivity Loss during Irradiation, $\Delta\rho^{cycle}$

At the first order, and neglecting the cross-section variation during irradiation (which is a good approximation for fast neutron systems), we can write:

$$\Delta\rho^{cycle} = \sum_K \Delta n^K \rho_K \tag{17}$$

where:

$$\Delta n^K = n_F^K - n_0^K \tag{18}$$

and ρ_K is the reactivity per unit mass associated to the isotope K.

The related sensitivity coefficients S_j^{cycle} associated to the variation of a σ_j, are given by:

$$S_j^{cycle} = \frac{\sigma_j}{\Delta\rho^{cycle}} \frac{\partial \Delta\rho^{cycle}}{\partial \sigma_j} = \frac{\sigma_j}{\Delta\rho^{cycle}} \left(\sum_K \frac{\partial n^K}{\partial \sigma_j} \cdot \rho_K + \sum_K \Delta n_K \frac{\partial \rho_K}{\partial \sigma_j} \right) \tag{19}$$

Using the formulations of Sec. 1.1. and Sec. 1.3., we obtain:

$$S_j^{cycle} = \sum_K \frac{\rho_K}{\Delta\rho^{cycle}} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \quad dt + \left\{ \frac{1}{I_f^p} \left\langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \right\rangle - \frac{1}{I_f} \left\langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \right\rangle \right\} \tag{20}$$

where the index “p” refers to the core state at $t = t_F$.

1.5 Case of a neutron source (e.g. at fuel fabrication)

A neutron source $NS_{t=tF}$ at $t = t_F$ can be defined as:

$$NS_{t=t_F} = \sum_i P_i n_{i,t=t_F} \tag{21}$$

where P_i is the neutron production cross-section (e.g. by spontaneous fissions). The sensitivity coefficients are:

$$S_j^i = P_i \cdot \frac{\partial n_F^i}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^i} = \frac{P_i}{n_F^i} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \, dt \tag{22}$$

where effects due to P_i cross-section variations are supposed to be negligible.

1.6. Decay Heat

The decay heat is defined as:

$$H(t) = \sum_K \lambda_K Q_K n_K(t) \tag{23}$$

where for each isotope K, λ_K are the decay constants, Q_K the heat released in decay reaction and $n_K(t)$ are the nuclide densities at time t. The equations for $n_K(t)$ are the classical ones:

$$\begin{aligned} \frac{dn_K(t)}{dt} = & \sum_F \gamma_{K,f} \tau_f + \sum_j n_K(t) \tau_j b_{j \to K} + \\ & + \sum_i n_i(t) \lambda_i b_{i \to K} - \tau_K n_K(t) - \lambda_K n_K(t) \end{aligned} \tag{24}$$

Or in a more compact form:

$$\frac{dn_k(t)}{dt} = b_k + \sum_{j=1}^{K-1} C_{kj} n_j(t) - C_{kk} n_k(t) \tag{25}$$

where $\gamma_{K,f}$ are the fission yields for fissionable isotope f, τ are microscopic reaction rates and $b_{j \to k}$ are branching ratios. This is an inhomogeneous Bateman-type equation that defines the appropriate nuclide field. The uncertainty on H(t) is obtained by combining the appropriate derivatives of H with respect to λ, Q and n, and accounting for possible correlations. As far as variations of the n_K terms, they can be evaluated using the perturbation techniques indicated in Sec 1.3. A specific feature is represented by the variation of the fission yields γ, i.e., by the variation of the "source" term b_K in Eq. (25).

The relative sensitivity coefficients corresponding to the decay heat at $t = t_x$ are given by:

$$S_K^{\gamma} = \tau_f \frac{\partial n_{t=t_x}^K}{\partial \gamma_{K,f}} \cdot \frac{\gamma_{K,f}}{n_{t=t_x}^K} = \frac{\tau_f}{n_{t=t_x}^K} \int_0^{t_x} \underline{n}^* \gamma_{K,f} \, dt \tag{26}$$

1.7. The Effective Fraction of Delayed Neutrons

The effective fraction of delayed neutrons, $\hat{\beta}_{eff}$, is defined by the following equation:

$$\hat{\beta}_{eff} = \sum_m \hat{\beta}_{eff}^m \tag{27}$$

where $\hat{\beta}_{eff}^m$ is the effective delayed neutron fraction of fissile material m. For each fissile material m, $\hat{\beta}_{eff} = \sum_i \hat{\beta}_i$, where $\hat{\beta}_i$, the effective fraction for the precursor group *i*, is expressed as follows:

$$\hat{\beta}_i = \frac{\left\langle \chi_i^d \underline{\Phi}^*, \beta_i \nu^d \Sigma_f \underline{\Phi} \right\rangle}{\left\langle \underline{\Phi}^*, F\underline{\Phi} \right\rangle} = \\ = \frac{\beta_i \int \left[\chi_i^d(E) \underline{\Phi}^*(r,E,\Omega) \right] \left[\nu^d(E') \Sigma_f(r,E') \underline{\Phi}(r,E',\Omega') \right] dr}{\left\langle \underline{\Phi}^*, F\underline{\Phi} \right\rangle} \tag{28}$$

where:

ν^d is the number of delayed neutrons emitted by fission;

χ_i^d is the delayed neutron spectrum for the group *i*;

β_i is fraction of delayed neutrons from the group *i*.

Using the Generalized Perturbation Theory, the sensitivity coefficients for $\hat{\beta}_{eff}$, including both the "direct" (i.e. related to the delayed neutron parameters) and the "indirect" effect, are given by:

$$S_j^{\hat{\beta}} = \frac{\partial \hat{\beta}_{eff}}{\partial \beta_i}\frac{\beta_i}{\hat{\beta}_{eff}} + \frac{\partial \hat{\beta}_{eff}}{\partial \chi_i^d}\frac{\chi_i^d}{\hat{\beta}_{eff}} + \frac{\partial \hat{\beta}_{eff}}{\partial \sigma_j}\frac{\sigma_j}{\hat{\beta}_{eff}} =$$
$$= \frac{\partial \hat{\beta}_{eff}}{\partial \beta_i}\frac{\beta_i}{\hat{\beta}_{eff}} + \frac{\partial \hat{\beta}_{eff}}{\partial \chi_i^d}\frac{\chi_i^d}{\hat{\beta}_{eff}} + \frac{\sigma_j}{\hat{\beta}_{eff}}\left\{\left\langle \underline{\Psi}^*, \sigma_j \underline{\Phi}\right\rangle + \left\langle \underline{\Psi}, \sigma_j \underline{\Phi}^*\right\rangle\right\} \tag{29}$$

where $\underline{\Psi}^*$ and $\underline{\Psi}$ ("generalized importance functions") are the solution of the following equations:

$$(A^* - F^*)\underline{\Psi}^* = \frac{\beta_i \left[\underline{\Phi}^* \chi_i^d\right] \nu^d \Sigma_f(r,E)}{\left\langle \chi_i^d \underline{\Phi}^*, \beta_i \nu^d \Sigma_f \underline{\Phi}\right\rangle} - \frac{\left[\underline{\Phi}^* \chi\right] \nu\Sigma_f(r,E)}{\left\langle \underline{\Phi}^*, F\underline{\Phi}\right\rangle} \tag{30}$$

$$\left(A - \frac{1}{K}F\right)\underline{\Psi} = \frac{\left[\beta_i \nu^d \Sigma_f \underline{\Phi}\right]\chi_i^d(E)}{\left\langle \chi_i^d \underline{\Phi}^*, \beta_i \nu^d \Sigma_f \underline{\Phi}\right\rangle} - \frac{\left[\nu\Sigma_f \underline{\Phi}^*\right]\chi}{\left\langle \underline{\Phi}^*, F\underline{\Phi}\right\rangle} \tag{31}$$

1.8. The φ^* Parameter

The φ^* parameter is defined for an external source-driven system as the ratio of the average external source importance to averaged fission neutron importance:

$$\phi^* = \frac{\left\langle \underline{\Phi}^* S\right\rangle}{\langle S\rangle} \Bigg/ \frac{\left\langle \underline{\Phi}^*, F\underline{\Phi}\right\rangle}{\langle F\underline{\Phi}\rangle} = \left(\frac{1}{K_{eff}} - 1\right) \Bigg/ \left(\frac{1}{K_S} - 1\right) \tag{32}$$

where $K_{eff} = \dfrac{\left\langle \underline{\Phi}^*, F\underline{\Phi}\right\rangle}{\left\langle \underline{\Phi}^*, A\underline{\Phi}\right\rangle}$, $K_S = \dfrac{\langle F\underline{\Phi}\rangle}{\langle A\underline{\Phi}\rangle}$ and $\underline{\Phi}$ is the solution of the inhomogeneous equation with external source S:

$$A\underline{\Phi} = F\underline{\Phi} + S. \tag{33}$$

Equation (32) is a special case of a real and the adjoint flux functional ratio I_S for which a GPT has also been established (Ref. 5).

For that case the sensitivity coefficients are given by:

$$S_j^{\phi^*} = \frac{\partial \phi^*}{\partial \sigma_j}\frac{\sigma_j}{\phi^*} = \frac{\sigma_j}{\phi^*}\left\{\left\langle \underline{\Psi}^*, \sigma_j \underline{\Phi}\right\rangle + \left\langle \underline{\Psi}, \sigma_j \underline{\Phi}^*\right\rangle\right\} \tag{34}$$

where $\underline{\Psi}^*$ and $\underline{\Psi}$ ("generalized importance functions") are the solution of the following equations:

$$M^*\underline{\Psi}^* = -\frac{\nu\Sigma_f(r,E)\left\langle \underline{\Phi}^*, \underline{\chi}\right\rangle}{\left\langle \underline{\Phi}^*, F\underline{\Phi}\right\rangle} + \frac{\nu\Sigma_f(r,E)}{\left\langle F\underline{\Phi}\right\rangle} \tag{35}$$

$$M\underline{\Psi} = \frac{S(r,E)}{\left\langle \underline{\Phi}^* S\right\rangle} - \frac{\chi(E)\left\langle \underline{\nu\Sigma}_f \underline{\Phi}\right\rangle}{\left\langle \underline{\Phi}^*, F\underline{\Phi}\right\rangle} \tag{36}$$

where we have explicitly introduced the energy and space dependent form of the fission operator, and $\nu\Sigma_f(E,r)$ (component of the vector $\underline{\nu\Sigma}_f$) is the macroscopic fission cross-section multiplied by the prompt neutron fraction at energy E and space point r and $\chi(E)$ (component of the vector $\underline{\chi}$) is the fraction of the fission spectrum at energy E; the brackets $\langle,\rangle$ indicate integration over energy and space.

1.9 Perturbation of the source term

An example is related to the γ-heating of a material j :

$$H_\gamma^j = < \underline{K}_\gamma^j \underline{\phi}_\gamma >$$

The photon flux $\underline{\phi}_\gamma$ is the solution of the following inhomogeneous equation :

$$M_\gamma \underline{\phi}_\gamma = \underline{S}_{(n\to\gamma)}$$

where $M\gamma$ is the Boltzmann operator for the transport of γ, and $\underline{S}_{(n\to\gamma)}$ is the photon source due to neutron reactions. At a photon energy E_γ, S is given by :

$$S(E_\gamma) = \sum_K \int \sigma_k(E_n) P_k(E_n \rightarrow E_\gamma) \phi_n(E_n) dE_n$$

where :

$\phi_n(E_n)$: neutron flux at neutron energy E_n

σ_k : neutron cross-section for γ-producing reaction type k

$P_k(E_n \rightarrow E_\gamma)$: γ-spectrum for γ issued of neutron reaction type k. These spectra are generally dependent on neutron energy E_n

To compute the sensitivity of $\boxed{H_\gamma^j}$ to uncertainties in the γ-source $\underline{S}_{(n\rightarrow\gamma)}$ it is necessary to define an "adjoint" equation :

$\boxed{M_\gamma^* \underline{\phi}_{\gamma,j}^* = \underline{K}_\gamma^j}$ $\underline{K}_\gamma^j$ being the photon KERMA for material j

to be coupled to the reference direct equation :

$$\boxed{M_\gamma \underline{\phi}_\gamma = \underline{S}_{(n\rightarrow\gamma)}}$$

Once more, one can obtain sensitivity coefficients of the type :

$$\frac{\partial H_\gamma^j}{H_\gamma^j} \Big/ \frac{\partial \underline{S}_{(n\rightarrow\gamma)}}{\underline{S}_{(n\rightarrow\gamma)}}$$

which in the case of the variation of the "neutron $\rightarrow$ photon source", are of the type :

$\left\langle \underline{\phi}_{\gamma j}^* \underline{S}_{(n\rightarrow\gamma)} \right\rangle$

which are independent of the perturbation, and than can be calculated only once.

2. Calculational Tools in the ERANOS code system

All the sensitivity calculations described above can be performed with the ERANOS code system (Ref.1), which allows to calculate homogeneous and inhomogeneous solutions of the Boltzmann equation and generalized importance functions, and to perform perturbation and uncertainty analysis. Specific modules in ERANOS allow generation of the source terms of the generalized importance equations and solution in two or three-dimensional of the finite-

difference diffusion or S_n transport equation, or of nodal variational transport equations. A fundamental mode removal algorithm is applied when solving the generalized importance equations for sources that are orthogonal to the homogeneous solutions. Procedures that manipulate different perturbation modules are used to generate the sensitivity coefficients related to reactivity coefficients.

The discrete ordinate module BISTRO (Ref.6) in ERANOS can be used to perform flux and generalized importance function calculations. In order to avoid problems related to S_n negative solutions that are present for instance in the case of reaction rate ratios importance calculations, ERANOS uses a special procedure that allows separately calculating the generalized importance for the positive and negative contributions and combining them at the level of the perturbation or sensitivity coefficient computation .

3. Ancillary calculations: uncertainty analysis and experiment representativity factors

Uncertainty evaluation and experiment representativity factors are computed in ERANOS with covariance matrices provided in different general formats.

3.1 Uncertainty analysis

The uncertainties associated to the cross-section can be represented in the form of variance-covariance matrix:

$$D_\sigma = \begin{pmatrix} d_{11} & d_{12} & \cdots & d_{1J} \\ d_{12} & d_{22} & \cdots & d_{2J} \\ \cdots & \cdots & \cdots & \cdots \\ d_{1J} & d_{2J} & \cdots & d_{JJ} \end{pmatrix} \qquad (37)$$

where the elements d_{ij} represent the expected values related to the parameters σ_j, and σ_i.

The variance of Q can then be obtained as:

$$\mathrm{var}(Q) = \sum_{j.i}^{J} S_j S_i d_{ij}$$

3.2 Expriment representativity factors

In order to plan for specific experiments able to reduce uncertainties on selected design parameters, a formal approach, initially proposed by L. Usachev (Ref.7) has been applied by Palmiotti and Salvatores (Ref.8) and further developed in by Gandini (Ref.9).
In the case of a reference parameter R, once the sensitivity coefficient matrix S_R and the covariance matrix D are available, the uncertainty on the integral parameter can be evaluated, as shown in Section 2.1, by the equation:

$$\Delta R_0^2 = S_R^+ D S_R \tag{38}$$

We can consider an integral experiment conceived in order to reduce the uncertainty ΔR_0^2. Let us indicate by S_E the sensitivity matrix associated with this experiment. If we call "representativity factor" the following expression:

$$r_{RE} = \frac{\left(S_R^+ D S_E\right)}{\left[\left(S_R^+ D S_R\right)\left(S_E^+ D S_E\right)\right]^{1/2}} , \tag{39}$$

it can be shown (Ref.7) that the uncertainty on the reference parameter R is reduced by:

$$\Delta R_0^{'2} = \Delta R_0^2 \cdot \left(1 - r_{RE}^2\right) \tag{40}$$

If more than one experiment is available, the Eq. (40) can be generalized. In the case of two experiments, characterized by sensitivity matrices S_{E1} and S_{E2} the following expression (Ref.9) can be derived:

$$\Delta R_0^{'2} = S_R^+ D' S_R = \Delta R_0^2 \left[1 - \frac{1}{1 - r_{12}^2}\left(r_{R1} - r_{R2}\right)^2 - \frac{2}{1 + r_{12}} r_{R1} r_{R2}\right] \tag{41}$$

where D' is the new covariance matrix and

$$r_{12} = \frac{\left(S_{E1}^+ D S_{E2}\right)}{\left[\left(S_{E1}^+ D S_{E1}\right)\left(S_{E2}^+ D S_{E2}\right)\right]^{1/2}} \tag{42}$$

$$r_{R1} = \frac{\left(S_R^+ D S_{E1}\right)}{\left[\left(S_R^+ D S_R\right)\left(S_{E1}^+ D S_{E1}\right)\right]^{1/2}} \tag{43}$$

$$r_{R2} = \frac{\left(S_R^+ D S_{E2}\right)}{\left[\left(S_R^+ D S_R\right)\left(S_{E2}^+ D S_{E2}\right)\right]^{1/2}} \tag{44}$$

The approach outlined here can be used to plan optimized integral experiments to reduce uncertainties on a set of integral parameters of a reference system.
All the formulations shown above can be calculated with specific modules of the ERANOS code system.

4. ERANOS tools. Some examples

In this section some examples are given of practical algorithm implementation using ERANOS tools and procedures.

ERANOS tools for building the source term of the equations for the importance functions

~ IMPORTANCE_CALCULATION_SOURCE_CREATION

```
-> edl_source_importance
geometry  (edl_geometry)  flux  (edl_flux)
                                    !! value ...
  << response_cross_section 'respname' !!          >>1
                                    !! edl ...
  ! numerator << response_function ... >>1
  ! numerator << response_function ... >>1 dose
  ! numerator << response_function ... >>1 denominator
      <<->xnum ->xden>> << response_function ... >>1
  << functional ->functional >> ;
```

the edl in output for each energy group associates to each mesh point the corresponding σ (defined in the `'edl'` directory) or value (defined in the `'value'` directory) multiplied by the volume of the mesh.

creates a source as: $S(r,E)=\frac{\sigma(r,E)dV}{\langle\sigma(r,E)\Phi(r,E)\rangle}$

creates a source as: $S(r,E)=\sigma(r,E)dV$

creates a source as: $S(r,E)=\frac{\sigma_1(r,E)dV}{\langle\sigma_1(r,E)\Phi(r,E)\rangle}-\frac{\sigma_2(r,E)dV}{\langle\sigma_2(r,E)\Phi(r,E)\rangle}$

gives the integral over space and energy of the source multiplied by the flux given in `'edl_flux'`: $\langle S(r,E)\Phi(r,E)\rangle$

```
! set data 1
! set data 2

!! set data 1
!! set data 2

<< set data >>0

<< set data >>1

<< set data >>
```

`set data n` are exclusive: one and only one must exist;

`set data n` are optional: they may exist all together and at least one must exist;

`set data` may be given 0 or n times;

`set data` may be given 1 or n times;

`set data` may be given 0 or 1 time.

ERANOS tools for building the source term of the equations for the importance functions

~ NORME_CALCULATION

it allows to calculate linear integrals, such as <SΦ>, where S can be either a cross-section or any source defined on the geometry grid, Φ is a scalar flux, either direct or adjoint.

Can be also used to calculate bilinear integrals, if S is function of the flux.
For instance, if $S_g = [\chi \Phi^*] \nu_g \Sigma_{f,g} dV$ **with g = 1…NG, NORME_CALCULATION can perform the calculation of < Φ*, F Φ>.**

~ GENERALIZED_INTEGRAL

it allows to calculate:

- **linear integrals <SΦ$_1$>;**
- **bilinear integrals <[S$_1$ Φ$_1$] [S$_2$ Φ$_2$] >**

where S, S$_1$ and S$_2$ can be either a cross-section or any source defined on the geometry grid, Φ$_1$ and Φ$_2$ are scalar fluxes, either direct or adjoint.

ERANOS procedure for spectral index sensitivity analysis

Adjoint importance function determination

```
importance_calculation_source_creation ->edl_source_ind
   geometry (edl_geometry)  flux (edl_flux_dir)
   response_cross_section 'secnum'
      edl (edl_micro) (region_n) (reaction_n) isotope (isotope_n)
   response_cross_section 'secden'
      edl (edl_micro) (region_d) (reaction_d) isotope (isotope_d)
   numerator
      response_function 'secnum' point (point_r_n) (point_z_n)
   denominator ->xnum ->xden
      response_function 'secden' point (point_r_d) (point_z_d)
   functional ->fonc ;
```

Building the source term for the importance function equation: $\frac{\sigma_1(E)dV}{\langle\sigma_1\Phi\rangle} - \frac{\sigma_2(E)dV}{\langle\sigma_2\Phi\rangle}$

$xnum = \langle\sigma_1\Phi\rangle \quad xden = \langle\sigma_2\Phi\rangle$

```
fd_diffusion_matrix_coefficient ->edl_coefficient
   geometry  (edl_geometry)  macro (edl_macro)
   horizontal_mesh  1. 1.    transport anisotropy 1 ;

methode_resolution_diffusion ->edl_method
   coefficient (edl_coefficient)  no_print
   plane alternating_direction_implicit calculation ;

direction_cosine_and_weight_creation ->edl_weights_directions
   section_set 'standard' ;

rectangular_sn_transport_iteration  ->edl_psi_adj
   angular_flux                     ->edl_psi_adj_ang
   method      (edl_method)
   coefficient (edl_coefficient)
   source      (edl_source_ind)
   direction   (edl_weights_directions)
   differencing_scheme diamant_pur
   harmonic     direct (edl_flux_dir)  adjoint (edl_flux_adj)
   calculational_parameter
      outer_iteration  maximum_number  50
               integral_convergence         1.e-5
               local_convergence            1.e-5
      inner_iteration  maximum_number  25
   no_scale  acceleration  diffusion diffusion_iteration 20
   variable_spectrum  calculation adjoint  moment_storage yes ;
```

Adjoint importance calculation:

$$\left(A^* - \frac{1}{K}F^*\right)\Psi^* = \frac{\sigma_1(E)dV}{\langle\sigma_1\Phi\rangle} - \frac{\sigma_2(E)dV}{\langle\sigma_2\Phi\rangle}$$

In transport approximation, the method `'diamant_pur'` must be used: the method `'diamant_teta 0.9'` is not appropriate because the source term could have negative values.

The option `'harmonic'` also prevent the use of the method `'diamant_teta 0.9'` (fix-ups would be also performed when the sign of the real solution is changing).

Inhomogeneous adjoint calculation: recommendation `'no_scale'`.

Indirect term

```
cross_section_variation_creation ->edl_cross_section_variation
   title         'cross_section variation'
   micro         (edl_micro)
   medium        (edl_medium)
   section_set   full
   isotope       one_by_one   partial (sensitivity_corp_list) ;
```

standard cross-section variation (100%) for sensitivity analysis.

```
->dispersion_matrix  ;
pour ->i (rep(sensitivity_corp_list()))  ;
   ->dispersion_matrix (dispersion_matrix) isotope
sensitivity_corp_list(i)
                 'capture'     rep(ng,1.00)
                 'fission'     rep(ng,1.00)
                 'nu'          rep(ng,1.00)
                 'elastique'   rep(ng,1.00)
                 'inelastique' rep(ng,1.00)
                 'n,xn'        rep(ng,1.00)
finpour ;

dispersion_matrix_creation ->edl_dispersion_matrix
   title  'dispersion matrix for sensitivity analysis'
   group (ng)
   deviation_standard (dispersion_matrix) ;
```

Dispersion matrix creation for sensitivity analysis: (diagonal terms = 1; 'off-diagonal' terms = 0).

For diffusion calculations add: `'transport' rep(ng,1.00)`

```
transport_perturbation_integral ->edl_perturbation_integral
      angular_flux  (edl_flux_dir_ang) (edl_psi_adj_ang)
      macro         (edl_macro)
      geometry      (edl_geometry)
      full ;

sensitivity_analysis   ->edl_indirect_sensitivity
   dispersion_matrix   (edl_dispersion_matrix)
   variation           (edl_cross_section_variation)
   integral            (edl_perturbation_integral)
   transport
   title ('*** sensitivity index '/(reaction_n)/' '/(isotope_n)/
          ' / '/(reaction_d)/' '/(isotope_d)/' ***')
   diffusion_coefficient_variation  approximate
   normalization_integral           input_value 1.00
   calculational_domain             full ;
```

Calculation of the indirect term in the sensitivity coefficient formula:

$$\frac{\sigma}{R}\left\langle \Psi^{*}, \left(\frac{\partial A}{\partial \sigma} - \frac{1}{K}\frac{\partial F}{\partial \sigma}\right)\Phi \right\rangle$$

For diffusion calculations: `'diffusion correction_transport micro(edl_micro)'.`

No normalization is performed on the sensitivity coefficients.

Direct term: $(\sigma_l\Phi)_{i,g,d}\,dV \,/\, \langle\sigma_l\Phi\rangle$

```
by_group_flux_creation
   flux (edl_flux_dir)  micro (edl_micro)  position (point_r_n) (point_z_n)
   title  'flux by group numerator' ->edl_flux_by_group_n ;
```

Φ_g g = 1 … NG
at the point (point_r_n) (point_z_n)

```
sample_macro ->sample_macro_n
   type (reaction_n)  section_set_micro (edl_micro) (region_n)
   sample (edl_medium)  isotope (isotope_n)  proportion  value 1.00 ;

by_group_value_creation_with_input_data ->edl_macro_by_group_n
   title  'direct sensitivity numerator'
   by_group_value (sample_macro_n)  micro (edl_micro) ;
```

$\sigma_{isotope\_n,\ reaction\_n,\ g}$ g = 1 … NG
at the point (point_r_n) (point_z_n)

```
by_group_value_operation
   (edl_macro_by_group_n) (edl_flux_by_group_n)
   produit ->edl_rate_by_group_n ;
```

$\sigma_{isotope\_n,\ reaction\_n,\ g} \cdot \Phi_g$ g = 1 … NG

```
(edl_rate_by_group_n) on_valgre group_value ->tpg ;
->total_n somme(tpg) ;  ->tpg (tpg/total_n) ;
(edl_rate_by_group_n) on_valgre group_value tpg ;
```

Normalizing:
$\sigma_{isotope\_n,\ reaction\_n,\ g} \cdot \Phi_g$
g = 1 … NG to sum = 1.

```
sensitivity_edl_changing ->edl_intermediate_sensitivity
   initialization (edl_indirect_sensitivity)
   sommation_valeur_par_groupe (edl_rate_by_group_n)
   domain (region_n)  reaction (reaction_n)  isotope (isotope_n);
```

Adding direct term in correspondence of reaction_n of isotope_n in the region region_n.

Direct term: $-(\sigma_2\Phi)_{i,g,d}\,dV \,/\, \langle\sigma_2\Phi\rangle$

```
by_group_flux_creation
   flux (edl_flux_dir)  micro (edl_micro)  position (point_r_d) (point_z_d)
   title  'flux by group denominator' ->edl_flux_by_group_d ;
```

Φ_g g = 1 … NG
at the point (point_r_d) (point_z_d)

```
sample_macro ->sample_macro_d
   type (reaction_d)  section_set_micro (edl_micro) (region_d)
   sample (edl_medium) isotope (isotope_d)  proportion  value 1.00 ;

by_group_value_creation_with_input_data ->edl_macro_by_group_d
   title  'direct sensitivity denominator'
   by_group_value (sample_macro_d)  micro (edl_micro) ;
```

$\sigma_{isotope\_d,\ reaction\_d,\ g}$ g = 1 … NG
at the point (point_r_d) (point_z_d)

```
by_group_value_operation
   (edl_macro_by_group_d) (edl_flux_by_group_d)
   produit ->edl_rate_by_group_d ;
```

$\sigma_{isotope\_d,\ reaction\_d,\ g} \cdot \Phi_g$ g = 1 … NG

```
(edl_rate_by_group_d) on_valgre group_value ->tpg ;
->total_d somme(tpg) ;  ->tpg (tpg/total_d) ;
(edl_rate_by_group_d) on_valgre group_value tpg ;
```

Normalizing:
$\sigma_{isotope\_d,\ reaction\_d,\ g} \cdot \Phi_g$
g = 1 … NG to sum = 1

```
by_group_value_operation
   (edl_rate_by_group_d) (edl_rate_by_group_d)
   linear_combination ->edl_rate_by_group_d -0.5 -0.5 ;
```

In order to add as negative contribution.

```
sensitivity_edl_changing ->edl_total_sensitivity
   initialization (edl_intermediate_sensitivity)
   sommation_valeur_par_groupe (edl_rate_by_group_d)
   domain (region_d)  reaction (reaction_d)  isotope (isotope_d) ;

sensitivity_edition (edl_total_sensitivity) ;
```

Adding direct term in correspondence of reaction_d of isotope_d in the region region_d.

Additional ERANOS tools for building the source term of the equations for the importance functions

~ Pointers

```
(EDL_ADJOINT_FLUX)
ON_FINITE_DIFFERENCE ON_REC_FLUX ON_FLUX_AND_SOURCE_POINTER
ON_TOTAL_SOURCE(1) SOURCE ->SOURCE;
```

SOURCE is a vector that contains in each point *i* of the grid: $\sum_{NG}(\nu\Sigma_f)_{g,i}\Phi_{g,i}dV_i = [\nu\Sigma_f\Phi]_i dV_i$

```
(EDL_DIRECT_FLUX)
ON_FINITE_DIFFERENCE ON_REC_FLUX ON_FLUX_AND_SOURCE_POINTER
ON_TOTAL_SOURCE(1) SOURCE ->SOURCE;
```

SOURCE is a vector that contains in each point *i* of the grid: $\sum_{NG}(\nu\Sigma_f)_{g,i}\Phi_{g,i}dV_i = [\nu\Sigma_f\Phi]_i dV_i$ where V_i is the volume of the mesh associated to the point *i*.

```
(EDL_FLUX)
ON_FINITE_DIFFERENCE ON_REC_FLUX ON_FLUX_AND_SOURCE_POINTER
ON_FLUX(IG,1) FLUX ->FLUX;
```

FLUX is a vector giving the flux in each point *i* of the grid for the group IG.

```
(EDL_IMPORTANCE_CALCULATION_SOURCE_CREATION)
ON_FINITE_DIFFERENCE ON_REC_FLUX ON_FLUX_AND_SOURCE_POINTER
ON_SOURCE(IG,1,1) SOURCE ->SOURCE;
```

SOURCE is a vector extrapolated from the EDL obtained with e.g.

Building the source term for the importance function equation: $[\Phi^{*}\chi]\nu\Sigma_f(r,E)dV$

```
importance_calculation_source_creation ->edl_fission_source
geometry (edl_geometry) flux (edl_flux_dir_inh)
response_cross_section  'sigma' edl (edl_macro) 'fuel' 'nu*fission'
  numerator response_function 'sigma' section 'fuel'
  dose  functional ->fission_source_integrated ;
```

Creating the source term: $\nu\Sigma_f(r,E)dV$

```
flux_initialization  ->edl_flux_nul
  with_input_data  reperage cylindrique rz
  coordinate  r    0.    1   142.   60
  coordinate  z    0.    1   200.   81
  number_of_groups (ng) mesh_point centre
  scalar_flux 0.  external_source 0.  total_source 0. ;
```

Creation flux with 0 values everywhere to be used as initialization for `'edl_adjoint_importance_source'`.

```
= ->edl_adjoint_importance_source (edl_flux_nul) ;
  (edl_flux_adj)
  on_finite_difference on_rec_flux on_flux_and_source_pointer
         on_total_source(1) source ->chi_phi ;
  pour ->ig (rep(ng)) ;
  (edl_fission_source)
  on_finite_difference on_rec_flux on_flux_and_source_pointer
         on_source(ig,1,1) source ->nu_sigmaf_dv ;
         ->source_importance_adjointe  (chi_phi*nu_sigmaf_dv) ;
  (edl_adjoint_importance_source)
  on_finite_difference on_rec_flux on_flux_and_source_pointer
         on_source(ig,1,1) source source_importance_adjointe ;
  finpour ;
```

Building the term: $[\Phi^{*}\chi]\nu\Sigma_f(r,E)dV$

chi_phi: $\sum_{g=1}^{NG}\Phi_g^{*}\chi_g$

nu_sigmaf_dv: $\nu_g\Sigma_{f,g}dV$

edl_adjoint_importance_source: $\sum_{g=1}^{NG}\Phi_g^{*}\chi_g\cdot\nu_g\Sigma_{f,g}dV$

```
rectangular_sn_transport_iteration  ->edl_psi_adj
  angular flux                      ->edl_psi_adj_ang
  method (edl_method)  coefficient (edl_coefficient)
  source (edl_adjoint_importance_source) direction (edl_weights_directions)
  differencing_scheme diamant_teta 0.9
  calculational_parameter
    outer_iteration maximum_number 30
      integral_convergence         1.e-5
      local_convergence            1.e-5
    inner_iteration maximum_number 30
  no_scale  acceleration diffusion diffusion_iteration 20
  variable_spectrum  calculation adjoint  moment_storage no ;
```

Adjoint importance function calculation

`'diamant_teta 0.9'` is used for source terms positive everywhere.

Source-driven problem: no need to use the option `'harmonic'`.

Building the direct term : $\left([\chi\Phi^*]\nu\Sigma_f\Phi\right)_{i,g,d}dV \Big/ \langle\Phi^*, F\Phi\rangle$

```
pour  ->dom (rep(liste_domaines())) ;  pour  ->cor (rep(liste_corps())) ;
```

```
importance_calculation_source_creation ->partial_edl_reaction_nu
geometry (edl_geometry) flux (edl_flux_dir)
response_cross_section 'sigma' edl (edl_micro) (liste_domaines(dom))
          'nu*fission' isotope (liste_corps(cor))  medium (edl_medium)
  numerator response_function 'sigma' section (liste_domaines(dom))
  dose functional ->partial_reaction_nu ;
```

Creating the term: $\left(\nu\Sigma_f\right)_{i,g,d}dV$
i=isotope
g=energy group
d=domain

```
->aden_iso_dom   (rep(ng,0)) ;
pour  ->ig (rep(ng)) ;
= ->edl_direct_term (edl_flux_nul) ;
  (edl_flux_adj)
  on_finite_difference on_rec_flux on_flux_and_source_pointer
          on_total_source(1) source -> chi_phi ;
  (partial_edl_reaction_nu)
  on_finite_difference on_rec_flux on_flux_and_source_pointer
          on_source(ig,1,1) source -> nu_sigmaf_dv ;
          -> direct_term (chi_phi* nu_sigmaf_dv)  ;
  (edl_direct_term)
  on_finite_difference on_rec_flux on_flux_and_source_pointer
          on_source(ig,1,1) source direct_term ;
```

Building the term: $[\Phi^*\chi]\nu\Sigma_f(r,E)dV$

chi_phi: $\sum_{g=1}^{NG}\Phi_g^*\chi_g$

nu_sigmaf_dv: $\left(\nu\Sigma_f\right)_{i,g,d}dV$

edl_direct_term: $\sum_{g=1}^{NG}\Phi_g^*\chi_g\cdot\left(\nu\Sigma_f\right)_{i,g,d}dV$

```
norme_calculation
reaction_rate (edl_direct_term) (edl_flux_dir)  ->aden_ig_iso_dom ;
->aden_iso_dom(ig) (aden_ig_iso_dom) ;
finpour ;
```

Building the term: $\left\langle[\chi\Phi^*](\nu\Sigma_f\Phi)_{i,g,d}\right\rangle$

```
by_group_value_creation_with_input_data ->edl_sens_by_isotope_den
  title 'direct sensitivity by isotope denominator'
  by_group_value (aden_iso_dom/aden)  micro (edl_micro) ;
by_group_value_operation
  (edl_sens_by_isotope_den) (edl_sens_by_isotope_den)
  linear_combination ->edl_sens_by_isotope_den -0.5 -0.5 ;
sensitivity_edl_changing ->sens_beff_tot
  initialization (sens_beff_tot) sommation_valeur_par_groupe (edl_sens_by_isotope_den)
  domain (liste_domaines(dom))  reaction 'nu*fission'  isotope (liste_corps(cor)) ;
sensitivity_edl_changing ->sens_beff_tot
  initialization (sens_beff_tot) sommation_valeur_par_groupe (edl_sens_by_isotope_den)
  domain (liste_domaines(dom))  reaction 'fission'  isotope (liste_corps(cor)) ;
```

Adding the direct term to the indirect one.

aden = $\langle\Phi^*, F\Phi\rangle$
(previously calculated)

```
finpour ;  finpour ;
```

5. References

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